UNIVERSITY OF TECHNOLOGY, SYDNEY

Nanoparticle Transport Modelling in Saturated Porous Media

A dissertation submitted in partial satisfaction of the requirements for the degree
Doctor of Philosophy

in
Engineering Science with Specialization in Groundwater Modelling

by

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CERTIFICATE OF ORIGINAL AUTHORSHIP

I certify that the work in this thesis has not previously been submitted for a degree nor has it been submitted as part of requirements for a degree except as fully acknowledged within the text.

I also certify that the thesis has been written by me. Any help that I have received in my research work and the preparation of the thesis itself has been acknowledged. In addition, I certify that all information sources and literature used are indicated in the thesis.

Signature of Student:

Date: 01/04/2014

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It is with incredulity that I face the end of this very interesting and eventful journey. The time has come to express gratitude to those who made it such an enjoyable ride.

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Dedications

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Vita and publications

This document features the following papers, posters, and presentations, either accepted or submitted for consideration at the time of submission. The dissertation author was the primary investigator and author of these publications.

Mehrabi, S., Milne-Home, W., 2014, *Modelling the transport of cylindrical nanoparticles in saturated porous media*, Environmental modelling &software, under preparation.

Mehrabi, S., Milne-Home, W., 2014, *Reducing the uncertainty in nanoparticle transport modelling by inclusion of natural heterogeneity of the porous media*, International Journal of Hydrology Science and Technology, Submitted.

Mehrabi, S., Milne-Home, W., 2013, *Optimization of Nanoparticle Delivery to Subsurface Contaminated Zone,* the 4th International Conference on Nanotechnology: Fundamentals and Applications, Toronto, Ontario, Canada.

Mehrabi, S., Milne-Home, W., 2012, *Representation of Heterogeneity in Single Collector Efficiency Equation for Multi-Walled Carbon Nanotubes*, International Journal of Theoretical and Applied Nanotechnology (IJTAN), 1-75-86pp.

Mehrabi, S., Milne-Home, W., 2012, *The Importance of Particle Orientation in the Transport of Carbon Nanotubes through Porous Media*, IAH 2012 International Congress: Confronting Global Change, Niagara falls, Canada.

Mehrabi, S., Milne-Home, W., 2012, *Representation of Heterogeneity in Single Collector Efficiency Equation for Multi-Walled Carbon Nanotubes*, the 3rd International Conference on Nanotechnology: Fundamentals and Applications, Montreal, Quebec, Canada.

Mehrabi, S., 2011, *Groundwater Protection Using Advanced Modelling Techniques*, Innovative Solutions for Environmental Challenges (ISEC 2011), Southern Cross University, Lismore, QLD.

Mehrabi, S., Milne-Home, W., 2011, *Applications of Nano-Size Zero Valent Iron Particles for Groundwater Remediation in NSW,* NSW IAH Symposium 2011 - Uncertainty in Hydrogeology, Sydney, NSW.

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Abstract

This research deals with multi-scale descriptions of nano-colloidal transport in saturated porous media. Colloidal transport has been simulated, historically, by employing a pore-scale model. I argue that the use of such simulations on a continuum-scale where formulations are generally phenomenological, may be unsuitable if at all possible due to requirements for pore-scale parameterization.

I propose to up-scale the pore-scale equation by inclusion of natural heterogeneity of porous media which consequently substitutes the pore-scale parameters (often unobtainable in real cases) with continuum-scale parameters (measurable at field). This approach transforms the pore-scale formulation into a Darcy-scale formulation, making it usable for real-world simulations.

I demonstrate a closer agreement with experimental data once porous media's natural heterogeneity is considered compared with the use of a mean value for media grain size in the conventional methods. These results can be explained by noting the fact that hydraulic conductivity of a porous medium is not controlled by the coarser or the median size grains. Rather, it is the smaller grains which ultimately determine (or in other words, restrict) the permeability of any given porous medium.

By comparing various modelled scenarios, I also assess the magnitude of difference in predicted results which displays a significant divergence from the case where the porous medium is assumed to be homogeneous.

Finally I aim to estimate the uncertainty associated with scenarios A (Yao's equation) and B (Mehrabi_ Milne-Home equation) in the absence and presence of natural heterogeneity, respectively. The results showed a noticeable decrease of 9% to 87% in the uncertainty caused by the most prominent source of uncertainty in groundwater modelling; porous media's

heterogeneity. The uncertainty is generally lower closer to the contaminant release point and increases as the plume moves away from the source point. The more substantial improvements (reduction of uncertainty) was observed at selected point which were located further away from the release point.

A framework for the assessment of nanoparticle transport in aquifers follows in which the extent of movement is estimated based on available field measured data and the probabilities of various potential realizations can be measured. This will help provide a much needed set of information for the policy-making processes with regards to new and emerging contaminants including engineered nanoparticles.